CURRICULUM VITAE

Surname, firstname, patronymic	**Dr. Toropova Alla P. (Toropova Alla Petrovna)**
Brief service record	1986 - 1991 – Lecturer in Industry College, Uzbekistan 1991 - 1994 – PhD student in Tashkent State University, Uzbekistan 1994 – 1998 – scientific collaborator at the Institute of Geology & Geophysics of the Academy of Sciences Rep. Uzbekistan 1998 - 2007 senior scientific researcher at the Institute of Geology & Geophysics of the Academy of Sciences Rep. Uzbekistan 2007–up to present, invited scientist at Istituto di Ricerche Farmacologiche Mario Negri *IRCCS*, Milano, Italy
Scientific interest	Quantitative Structure–Property/Activity Relationships (QSPR/QSAR): modeling of endpoints such as toxicity, mutagenicity, HIV-1, as well as physicochemical properties; QSPR/QSAR analysis of nanomaterials; inorganic and organometallic compounds. Web design: http://www.insilico.eu/CORAL
Scientific degree	**Ph.D. in chemistry** (1998)
Membership in Editorial Board of scientific journals	2025, **Guest Editor** of an issue of Toxics (impact factor =4.1); Special issue: "Computational Toxicology: Exposure and Assessment". This special issue belongs to the section "Novel Methods in Toxicology Research". https://www.mdpi.com/journal/toxics/special_issues/3V01KO33IB 2025, **Guest Editor** of an issue of Discover Nano; Special issue: " QSPR/QSAR for Nano Phenomena: Recent Developments, Applications, and Ideas". https://link.springer.com/collections/fbfaifjhje 2024, **Guest Editor** of an issue of Toxics (impact factor =4.1); Special issue: " Advances in Computational Toxicology and Their Exposure". This special issue belongs to the section "Novel Methods in Toxicology Research". https://www.mdpi.com/journal/toxics/special_issues/Q5K6T2BTG0 2021, **Guest Editor** of an issue of Frontiers in Bioscience-Landmark (impact factor = 4.009); Special issue: "Drug-induced Diseases: Computational Approaches for Averting It". https://www.imrpress.com/journal/FBL/special_issues/1396741473864962049 2021, **Guest Editor** of an issue of Molecules (impact factor =4.6); Special issue: "QSAR and QSPR: Recent Developments and Applications II"; this special issue belongs to the section "Computational and Theoretical Chemistry". https://www.mdpi.com/journal/molecules/special_issues/QSAR_QSPR_II 2021, **Guest Editor** of an issue of Chemistry; Special issue: "QSAR and QSPR: Recent Developments and Applications 2021 "; this special issue belongs to the section "Theoretical Chemistry". https://www.mdpi.com/journal/chemistry/special_issues/QSAR_QSPR_Applications 2020, **Guest Editor** of an issue of Mini-Reviews in Medicinal Chemistry (MRMC) (impact factor =3.86); Special issue: “Medicinal Chemistry and Computational Chemistry: Mutual Influence and Harmonization”; Vol. 20, No. 14. 2018, **Guest Editor** of an issue of International Journal of Quantitative Structure-Property Relationships; Special issue: “Applications of QSPR/QSAR in Toxicology, Ecology, and Drug Discovery: Problems and Solutions”; Volume 3, Issue 2. 2017, **Guest Editor** of an issue of Current Drug Metabolism (impact factor =3.731); Special issue: “Impact of Drug Metabolism and its Relevance upon Drug Discovery”; Vol. 18, No. 12 2015, **Guest Editor** of an issue of Current Topics in Medicinal Chemistry (CTMC) (impact factor =3,295); Special issue: “From Chemoinformatics to Nanoinformatics: New tools for Drug Discovery and Nanoparticles Design in Medicinal Chemistry”; Vol. 15, No. 18.

Member of the Advisory Editorial Board of the journal " Current Protein & Peptide Science" http://www.eurekaselect.com/node/619/current-protein-peptide-science/editorial-board
Member of Editorial Review Board of the Journal of Nanotoxicology and Nanomedicine(JNN) http://www.igi-global.com/journal/journal-nanotoxicology-nanomedicine-jnn/126553
Member of the Editorial Board of the journal " Molecules" https://www.mdpi.com/journal/molecules/editors
Member of the Associate Editors **of the journal " Frontiers in Pharmacology" in the section Predictive Toxicology** https://www.frontiersin.org/journals/pharmacology/editors?section=Predictive%20Toxicology

Referee in

Nanoscale
Chemosphere
RSC Advances
Computers in Biology and Medicine
Medicinal Chemistry Research
Combinatorial Chemistry & High Throughput Screening
Journal of Chemical Information and Modeling
Current Topics in Medicinal Chemistry
Drug Research
Chemometrics and Intelligent Laboratory Systems
Chemical Biology and Drug Design
International Journal of Quantitative Structure-Property Relationships (IJQSPR)
Bioorganic and Medicinal Chemistry

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Participation in conferences and workshops

April 11, 2023-MRS Spring Meeting & Exhibit in San Francisco. https://www.mrs.org/meetings-events/spring-meetings-exhibits/2023-mrs-spring-meeting/call-for-papers/presentations/detail/2023_mrs_spring_meeting/3838685-202304110845
September 21 – 23, 2022, 28th Annual Meeting of the Slovenian Chemical Society, Portorose, Slovenia.
November 11-12, 2021, Nanosafety workshop - From Molecules to Public Health. Portugal, Braga.
26-30 May 2019, The SETAC Europe 29th Annual Meeting, Helsinki, Finland.
June 24, 2016, XLI ELBA Nanoforum on Emerging Lines of Collaborative Russians/Italians Research, Pradalunga (Bergamo), Italy
5–15 December 2015. MOL2NET, International Conference on Multidisciplinary Sciences, C: Polymers, Materials, and Nanosciences. http://sciforum.net/conference/MOL2NET-1/MOL2NET-c
November 4-6, 2015, CompNanoTox-2015, Malaga, Spain
7 - 11 July 2015, 12th International Conference on Nanosciences (NN15). Thessaloniki, Greece
April 29, 2015, CALEIDOS (Final Workshop- 2015), Milan , Italy
June 16-20, 2014, QSAR 2014, Milan, Italy
June 4-6, 2013, Harmonisation meeting with representatives of other projects in the NMP.2012.1.3-2 Programme "Modelling toxicity behaviour of engineered nanoparticles": ModEnpTox, Modern, NanoPuzzles, PreNanoTox in Brussels, Belgium.
May, 2011, SETAC , Milan, Italy
March, 2011, Orchestra, Milan, Italy
September, 2009, VII World Congress on Alternatives & Animal Use in the Life Sciences, Rome, Italy (poster)
May, 2009, SETAC, Goteborg, Sweden
March, 2008, SCARLET – Istituto di Ricerche Farmacologiche Mario Negri, Milan, Italy

Participation in International scientific grants

CAESAR (EC Project no. 022674 - SSPI)
OSIRIS (n. 037017 -GOCE)
ANTARES (Grant Agreement LIFE08 ENV/IT/00435)
PROSIL (projectLIFE12ENV/IT/000154)
Federchimica-AISPEC
NanoBRIDGE (Grant Agreement: PIRSES-GA-2011-295128)
NanoPUZZLES(EC Project Reference:309837)
PreNanoTox (EC Project Reference: 309666)
CALEIDOS (Grant Agreement LIFE 11 ENV/IT/000295)
EC project PeptiCAPS (Project Reference: H2020-686141)
LIFE-COMBASE (LIFE15 ENV/ES/000416)
EC project EU-ToxRisk- H2020-681002
EFSA contract (NP//EFSA/AFSCO/2016/1)
LIFE-VERMEER contract (LIFE16 ENV/IT/000167)
LIFE-CONCERT contract (LIFE17 GIE/IT/000461)

Characterization of Dr. Toropova A.P. by Google Scholar Citations
https://scholar.google.com/citations?user=0W8tjIAAAAAJ&hl=it

Citation indices	All	Since 2021
Citations	8390	3635
h-index	46	28
i10-index	230	134

Characterization of Dr. Toropova A.P. by SCOPUS database
http://www.scopus.com/authid/detail.url?authorId=6701335146
h-Index =42 (i.e., there are 42 articles that are cited 42 or more times)

Year	The number of published articles and chapters	The total number of citations up to now
2026	6 +2(in press)	155
2025	18	506
2024	9	491
2023	34	738
2022	19	542

The total number of citations (SCOPUS) is 6907 (May 22, 2026)

PUBLICATION LIST OF ALLA P. TOROPOVA
Chapters in Books and other publications:

- A.P. Toropova, A.A. Toropov, E. Benfenati, **Chapter 9**. Simulation of physicochemical and biochemical behavior of nanoparticles under various experimental conditions. **In**: *Roy, K., Banerjee, A. (eds)* Cheminformatic Modeling and Data Gap Filling for a Green and Sustainable Environment, **2026**, 1st Edition - May 1, 2026. Elsevier. eBook ISBN: 9780443364754. https://shop.elsevier.com/books/cheminformatic-modeling-and-data-gap-filling-for-a-green-and-sustainable-environment/roy/978-0-443-36474-7

- Toropov, A.A., Toropova, A.P., Roncaglioni, A., Benfenati, E. ***Chapter 19***. Quasi-SMILES as a tool for simulation of endpoints related to nanomaterials. ***In****: Alfaro-Moreno, E., Murphy, F. (eds)* Nanosafety. **2025**, pp 531–557. Springer, Cham. https://doi.org/10.1007/978-3-031-93871-9_19

- N. Fjodorova, M. Novič, K. Venko, B. Rasulev, M. Türker Saçan, G. Tugcu, S. Sağ Erdem, A.P. Toropova, A.A. Toropov, ***Chapter 6***. Applications of Predictive Modeling for Fullerenes. **In:** *Roy, K., Banerjee, A. (eds)* Materials Informatics II. Challenges and

Advances in Computational Chemistry and Physics, **2025**, vol. 40, pp. 133–151. Springer, Cham. https://doi.org/10.1007/978-3-031-78728-7_6

- **In Book**: *Toropova, A.P., Toropov, A.A. (eds).* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol. 33, pp.1-467. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4

- Toropov, A.A., Raskova, M., Raska, I., Toropova, A.P.
Chapter 1. Fundamentals of Mathematical Modeling of Chemicals Through QSPR/QSAR. **In:** *Toropova, A.P., Toropov, A.A.* (*eds*) QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol. 33, Pages 3–24. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_1

- Toropov, A.A., Toropova, A.P.
Chapter 3. Application of SMILES to Cheminformatics and Generation of Optimum SMILES Descriptors Using CORAL Software. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 57-82. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_3

- Kudyshkin, V.O., Toropova, A.P.
Chapter 7. Building Up QSPR for Polymers Endpoints by Using SMILES-Based Optimal Descriptors. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 167-187. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_7

- Behera, S.A., Toropova, A.P., Toropov, A.A., Achary, P.G.R.
Chapter 9. Quasi-SMILES-Based Mathematical Model for the Prediction of Percolation Threshold for Conductive Polymer Composites. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 211-239. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_9

- Achary, P., Krishna, P., Toropova, A.P., Toropov, A.A.
Chapter 10. On the Possibility to Build up the QSAR Model of Different Kinds of Inhibitory Activity for a Large List of Human Intestinal Transporter Using Quasi-SMILES. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 241-268. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_10

- Toropova, A.P., Toropov, A.A.
Chapter 14. The CORAL Software as a Tool to Develop Models for Nanomaterials' Endpoints. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 351-371. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_14

- Toropov, A.A., Toropova, A.P., Leszczynska, D., Leszczynski, J.
Chapter 16. On Complementary Approaches of Assessing the Predictive Potential of QSPR/QSAR Models. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry

and Physics, **2023**, vol 33, Pages 397-420. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_16

- Nilima R. Das, Tripti Sharma, Ayeshkant Mallick, Alla P. Toropova, Andrey A. Toropov, and P. Ganga Raju Achary,
Chapter 32. Computational Approach in Designing and Development of Novel Inhibitors of AKR1C1. **In Book**: Tripti Swarnkar, Srikanta Patnaik, Indian Institute of Technology (IIT), *Sanjay Misra, Siksha O. (Eds)*, Ambient Intelligence in Health Care: Proceedings of ICAIHC 2022: 325-339. (Smart Innovation, Systems and Technologies, vol. 317). Springer; 1st ed. **2023** edition. https://doi.org/10.1007/978-981-19-6068-0

- Alla P. Toropova and Andrey A. Toropov,
Chapter 3. Use of the Monte Carlo Method to Build up QSPR/QSAR Models: Index of Ideality of Correlation and Correlation Intensity Index. **In Book**: *Thomas B. Hall (Ed.)*, Monte Carlo Methods: History and Applications. Series: Mathematics Research Developments. Nova, **2020**, pp.111-156. ISBN: 978-1-53617-723-7 https://novapublishers.com/shop/monte-carlo-methods-history-and-applications/

- Andrey A. Toropov, Alla P. Toropova, Alessandra Roncaglioni, and Emilio Benfenati,
Chapter 27. Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. **In Book**: *Orazio Nicolotti (ed.)*, Computational Toxicology: Methods and Protocols, Methods in Molecular Biology, **2018**, vol. 1800, pp. 573-583. https://doi.org/10.1007/978-1-4939-7899-1_27, © Springer Science+Business Media, LLC, part of Springer Nature

- Andrey A. Toropov and Alla P. Toropova,
Chapter 8. Improved Model for Biodegradability of Organic Compounds: The Correlation Contributions of Rings. **In Book**: *Bidoia E., Montagnolli R. (Eds)* Toxicity and Biodegradation Testing. Methods in Pharmacology and Toxicology. Humana Press, New York, NY. **2018**, pp. 147-183. DOI: 10.1007/978-1-4939-7425-2_8

- Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, Robert Rallo, Danuta Leszczynska and Jerzy Leszczynski,
***Chapter* 12**. Development of Monte Carlo Approaches in Support of Environmental Research. **In Book**: *Roy, K.* (*eds*) Advances in QSAR modeling. Advances in Computational Chemistry and Physics. Springer International Publishing AG, **2017,** Volume 24, pages 453-469.

- Alla P. Toropova, Andrey A. Toropov, Aleksandar M. Veselinović, Jovana B. Veselinović, Danuta Leszczynska, Jerzy Leszczynski,
Chapter 8. Quasi-Smiles as a novel tool for Prediction of Nanomaterials' endpoints. **In Book**: *Speck-Planche A.* (*eds*) Multi-Scale Approaches in Drug Discovery: From Synthetic Methodologies and Biological Assays to In Silico Experiments and Back. Elsevier Science & Technology Books, **2017,** pages 191-221. ISBN: 0081011296, 9780081011294

- Alla P. Toropova, P. Ganga Raju Achary, Andrey A. Toropov,
Chapter 59. Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al_2O_3 Nanoparticles. **In Book:** Pharmaceutical Sciences: Breakthroughs in Research and Practice (2 Volumes) **2017**, pages 1573-1584. DOI: 10.4018/978-1-5225-1762-7

- A.A. Toropov, A.P. Toropova, E. Benfenati, O. Nicolotti, A. Carotti, K. Nesmerak, A.M. Veselinović, J.B. Veselinović, P.R. Duchowicz, D. Bacelo, E.A. Castro, B.F. Rasulev, D. Leszczynska, J. Leszczynski,
Chapter 36. QSPR/QSAR Analyses by Means of the CORAL Software: Results, Challenges, Perspectives. **In Book**: Pharmaceutical Sciences: Breakthroughs in Research and Practice (2 Volumes) **2017,** pages 929-955. DOI: 10.4018/978-1-5225-1762-7

- Toropov A.A., Toropova A.P., Nesmerak K., Veselinović A.M., Veselinović J.B., Leszczynska D., Leszczynski J.,
Chapter 12. Development of the latest tools for building up "nano-QSAR": Quantitative features—property/activity relationships (QFPRs/QFARs). **In Book**: *J. Leszczynski, M.K. Shukla (Eds.)*. Practical Aspects of Computational Chemistry IV. Springer **2016**, pp. 353-396. DOI: 10.1007/978-1-4899-7699-4_12

- Toropov A.A., Toropova A.P. The CORAL software as spyglass to detect "coral reefs" in ocean of nanotechnologies. **2015**. *Available on the Atlas of Science* website: http://atlasofscience.org/the-coral-software-as-spyglass-to-detect-coral-reefs-in-ocean-of-nanotechnologies/#more-1267

- A.A. Toropov, A. P. Toropova, E. Benfenati, O. Nicolotti, A. Carotti, K. Nesmerak, A. M.Veselinovic, J. B. Veselinovic, P. R. Duchowicz, D. Bacelo, E. A. Castro, B. F. Rasulev, D. Leszczynska, J. Leszczynski,
Chapter 15. QSPR/QSAR analyses by means of the CORAL software: results, challenges, perspectives. **In Book**: *Roy, K. (Eds.)* Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment. **2015**, pp. 1-531. Hershey, PA: IGI Global. doi:10.4018/978-1-4666-8136-1 http://www.igi-global.com/book/quantitative-structure-activity-relationships-drug/120080

Articles in Impacted (or Peer-reviewed) Journals

2026:

1. Alla P. Toropova, Andrey A. Toropov, Sofia Mescieri, Alessandra Roncaglioni and Emilio Benfenati, Simulation of the impact of pesticides on pollinators under different conditions using correlation weighting of quasi-SMILES components together with the Index of Ideality of Correlation (IIC). Journal of Xenobiotics, 2026, 16(1), 10. https://doi.org/10.3390/jox16010010
2. Andrey A. Toropov, Alla P. Toropova, Simone Stefano, Alessandra Roncaglioni and Emilio Benfenati, Simulation of polydimethylsiloxane-water partition coefficients for organic compounds using the CORAL software. Structural Chemistry, Accepted Mar 15, 2026. https://doi.org/10.1007/s11224-026-02771-z
3. Benfenati E., Roncaglioni A., Iovine N., Toropov A., Toropova A., Ciacci A., Sartori L., Valerio M., Hobocienski B., Marusczyk J., Sacher O., Schwab C. H., 2026. Further development and update of EFSA's Chemical Hazards database: OpenFoodTox 3.0. EFSA supporting publication 2026:23(4):EN-10099. 104 pp. doi:10.2903/sp.efsa.2026.EN-10099
4. A.P. Toropova, A.A. Toropov, G. Selvestrel, N. Iovine, A. Roncaglioni & E. Benfenati. QSPR models for water solubility of organic compounds using correlation intensity index and Las Vegas algorithm, SAR and QSAR in Environmental Research, 37(4), 2026, 299-310. DOI: 10.1080/1062936X.2026.2659325. DOI: 10.1080/1062936X.2026.2659325
5. Toropova, A.P.; Toropov, A.A.; Raŝka, I., Jr.; Raŝkova, M.; Achary, P.G.R. QSAR Models for Sweetness: Can They Shape the Future of Nutritional Safety? Foods 2026, 15, 1481. https://doi.org/10.3390/foods15091481

6. Toropova, A.P.; Toropov, A.A.; Iovine, N.; Selvestrel, G.; Roncaglioni, A.; Benfenati, E. QSAR Models for Repeated Dose Toxicity in Rats Using the CORAL Software. Toxics 2026, 14, 338. https://doi.org/10.3390/toxics14040338
7. Andrey A. Toropov, Erika Colombo, Alla P. Toropova, Anna Lombardo, Edoardo Luca Viganò, Alessandra Roncaglioni and Emilio Benfenati, Simulation of chronic aquatic toxicity toward fish using the Las Vegas algorithm and the vector of ideality of correlation. Environmental Toxicology and Chemistry, Accepted May 18, 2026.

2025:

8. Iovine, N.; Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Simulation of the Long-Term Toxicity towards Bobwhite Quail (Colinus virginianus) by the Monte Carlo method. J. Xenobiot. 2025, 15, 3. https://doi.org/10.3390/jox15010003
9. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. In Silico Simulation of Daphnia magna immobilization exposed to mixtures of TiO_2 nanoparticles with inorganic compounds. J. Compos. Sci. 2025, 9, 16. https://doi.org/10.3390/jcs9010016
10. A. P. Toropova, A. A. Toropov, A. Roncaglioni, E. Benfenati, Monte Carlo simulation of aromatic molecules adsorption on multi-walled carbon nanotube surfaces using coefficient of conformism of a correlative prediction (CCCP). C-Journal of Carbon Research, 2025, 11, 7. https://doi.org/10.3390/c11010007
11. Andrey A. Toropov, Alla P. Toropova, Valentin O. Kudyshkin, Danuta Leszczynska, Jerzy Leszczynski, Application of monomer structures and fragments of local symmetry for simulation of glass transition temperatures of polymers. SAR and QSAR in Environmental Research, 2025, 36(1), 29–37. DOI: 10.1080/1062936X.2025.2453868
12. Aleksandar M. Veselinović, Alla P. Toropova, Andrey A. Toropov, Alessandra Roncaglioni, Emilio Benfenati, Las Vegas algorithm in the prediction of intrinsic solubility of drug-like compounds, Journal of Molecular Graphics and Modelling, 137, 2025,109004. https://doi.org/10.1016/j.jmgm.2025.109004
13. Shahram Lotfi, Shahin Ahmadi, Alla P. Toropova, Andrey A. Toropov, Monte Carlo approach to study the impact sensitivity of nitro compounds using correlation weights of the fragments of molecular structures. Scientific Reports, (2025) 15:11160. https://doi.org/10.1038/s41598-025-95129-0
14. Toropov, A.A.; Toropova, A.P.; Roncaglioni, A.; Benfenati, E. Semi-Correlations for the Simulation of Dermal Toxicity. Toxics 2025, 13, 235. https://doi.org/10.3390/toxics13040235
15. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Using the Coefficient of Conformism of a Correlative Prediction in simulation of cardiotoxicity. Toxics. 2025; 13(4):309. https://doi.org/10.3390/toxics13040309
16. Toropova, A.P.; Toropov, A.A.; Benfenati, E. Monte Carlo Simulation of Pesticide Toxicity for Rainbow Trout (*Oncorhynchus mykiss*) Using New Criteria of Predictive Potential. J. Xenobiot. 2025, 15, 82. https://doi.org/10.3390/jox15030082
17. Alla P. Toropova, Andrey A. Toropov, Alessandra Roncaglioni, Emilio Benfenati, In silico models of biological activities of peptides using the coefficient of conformism of a correlative prediction and the Las Vegas algorithm. Macromol 2025, 5(2), 27. https://doi.org/10.3390/macromol5020027
18. Shahin Ahmadi, Shahram Lotfi, Alla P. Toropova, Andrey A. Toropov, On some strange model for the impact sensitivity of nitro compounds obtained with Monte Carlo method. Chemical Physics Letters, 878, 2025, 142249. https://doi.org/10.1016/j.cplett.2025.142249
19. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. New QSPR/QSAR Models for Organic and Inorganic Compounds: Similarity and Dissimilarity. Inorganics 2025, 13, 226. https://doi.org/10.3390/inorganics13070226

20. Andrey A. Toropov, Alla P. Toropova, Valentin O. Kudyshkin, Emilio Benfenati, Danuta Leszczynska, Jerzy Leszczynski, Simulation peptide toxicity using the fragments of local symmetry in amino acid sequences, BioSystems, 256, 2025, 105554, https://doi.org/10.1016/j.biosystems.2025.105554
21. Shahram Lotfi, Shahin Ahmadi, Ali Azimi, Alla P. Toropova, Andrey A. Toropov, In Silico prediction of pesticide residue retention times in foods and vegetables using the Monte Carlo technique. Food Research International 221 (2025) 117479. https://doi.org/10.1016/j.foodres.2025.117479
22. Toropova, A.P.; Toropov, A.A.; Colombo, E.; Viganò, E.L.; Lombardo, A.; Roncaglioni, A.; Benfenati, E. Simulation of Fish Acute Toxicity of Pharmaceuticals Using Simplified Molecular Input Line Entry System (SMILES) Notation as a Representation of Molecular Structure. Int. J. Mol. Sci. 2025, 26, 9348. https://doi.org/10.3390/ijms26199348
23. Alla P. Toropova, Andrey A. Toropov, Ivan Raska Jr, Maria Raskova, Emilio Benfenati, Danuta Leszczynska, Jerzy Leszczynski, Chaos, Gambling, Simplicity: Simulation of nanoparticle delivery efficiency to organs of mice, In Silico Research in Biomedicine, 2025, 100105, https://doi.org/10.1016/j.insi.2025.100105

2024:

24. Alla P. Toropova and Andrey A. Toropov, The coefficient of conformism of a correlative prediction (CCCP): Building up reliable nano-QSPRs/QSARs for endpoints of nanoparticles in different experimental conditions encoded via quasi-SMILES. Science of the Total Environment 927 (2024) 172119. https://doi.org/10.1016/j.scitotenv.2024.172119
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Conferences and workshops

SCARLET – Istituto di Ricerche Farmacologiche Mario Negri– April 2-4, 2008
1.A.A. Toropov, A.P. Toropova, E. Benfenati
QSAR modeling of carcinogenicity and mutagenic potency by optimal SMILES-based descriptors **2.** E. Benfenati, A. Chana, A.A. Toropov, A.P. Toropova
QSAR modeling of carcinogenicity based on local attributes of SMILES and special codes of cycles 1st SETAC Europe Special Science Symposium 23-24 October 2008, Brussels
3. A. Chana, A.A. Toropov, A.P. Toropova, E. Benfenati, X.-K. Hu, H.-M. Hwang, B.F. Rasulev, T. Puzyn, J. Leszczynski QSAR modelling of biological activity by descriptors calculated with simplified molecular input line entry system (SMILES)

SETAC – Goteborg (Sweden) – May 2009
1. A.A. Toropov, A.P. Toropova and E. Benfenati

QSAR modelling of mutagenicity: the applicability domain definition and the estimation of predictive ability
2. A.A. Toropov, A.P. Toropova, X.-K. Hu, H.-M. Hwang, B.F. Rasulev, T. Puzyn, E. Benfenati, D. Leszczynska, and J. Leszczynski
QSAR model of toxicity towards *E.Coli* bacteria for nanosized oxides by SMILES-based optimal descriptors

VII World Congress on Alternatives & Animal Use in the Life Sciences – Italy, Rome, September, 2009
A.A. Toropov, A.P. Toropova, E. Benfenati
Additive smiles-based carcinogenicity models: a new approach to increase robustness and prediction

Orchestra March 2011, Milan, Italy
1. Alla. P. Toropova, Andrey A. Toropov, Emilio Benfenati, Giuseppina Gini, Danuta Leszczynska, Jerzy Leszczynski
QSAR modeling of toxicity of binary mixtures by CORAL software
2. Andrey A. Toropov, Alla. P. Toropova, Emilio Benfenati, Giuseppina Gini, Danuta Leszczynska, Jerzy Leszczynski
QSAR modeling of cytotoxicity of nanoparticles

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1. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Giuseppina Gini
SMILES-based QSPR model for Bioconcentration Factor
2. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Giuseppina Gini
QSAR for toxicity of aromatic aldehydes to Tetrahymena pyriformis using correlation weights of physicochemical situations
3. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Giuseppina Gini
QSAR models for toxicity of organic substances to Daphnia magna built up by using the CORAL freeware

QSAR 2014, June 16-20, 2014, Milan Italy
1. F. Pizzo, D. Gadaleta, A. Lombardo, A. A. Toropov, A. P.Toropova, S. E. Escher, O. Nicolotti, A. Carotti, E. Benfenati
Different Approaches for Modeling Repeated Dose Toxicity, Lecture
2. Alla P. Toropova, Andrey A. Toropov, Aleksandar M. Veselinović, Jovana B. Veselinović, Emilio Benfenati, Orazio Nicolotti, Angelo Carotti, Danuta Leszczynska, Jerzy Leszczynski Optimal descriptor as a translator of eclectic data into models for mutagencity of fullerene in different conditions, Poster
3.Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati
Quasi-QSPR/QSAR: reasons, tasks, results, Poster
4. V. H. Masand, A. P. Toropova, A. A. Toropov, D. T. Mahajan
QSAR Modeling of Anxiolytic Activity Taking into Account the Presence of Keto-Enol Tautomerism, Poster
5. V. H. Masand, A. A. Toropov, A. P. Toropova, D. T. Mahajan
The Monte Carlo Method as a Tool to Predict Anti-Malarial Activity of 4-Aminoquinolines, Poster

12th International Conference on Nanosciences (NN15). Thessaloniki, Greece, 7 - 11 July 2015
Manganelli, S., Leone, C., Toropov, A.A., Toropova, A.P., Benfenati, E. (2015): QSAR model for cytotoxicity of silica nanoparticles on human embryonic kidney cells. (poster presentation).

CompNanoTox2015. Malaga, Spain, 4-6 November 2015
Toropova, A.P., Toropova, A.A., Benfenati, E. (2015): Modelling nanomaterials with CORAL. (poster presentation).

The SETAC Europe 29th Annual Meeting, held on 26-30 May 2019 in Helsinki, Finland
E. Carnesecchi, A.A. Toropov, A.A. Toropova, N. Kramer, C. Svendsen, J. Dorne, E. Benfenati.
TU317: CORAL: innovative open source QSAR model for predicting acute contact toxicity of binary mixtures of plant protection products in honeybee (A. mellifera). (poster presentation).

Nanosafety workshop - From Molecules to Public Health (November 11-12, 2021, Portugal, Braga).
Andrey Toropov, Alla Toropova. Cheminformatics and in silico tools: What is Quasi-SMILES? How to use for nano-QSPR/QSAR?

28th Annual Meeting of the Slovenian Chemical Society (September 21 – 23, 2022, Portorose, Slovenia).
Natalja Fjodorova, Marjana Novič, Katja Venko, Bakhtiyor Rasulev, Melek Türker Saçan, Gulcin Tugcu, Safiye Sağ Erdem, Elifcan Çalışkan, Alla P. Toropova, Andrey A. Toropov.
Investigation of aquatic toxicity of fullerene derivatives using cheminformatics approach.

SB05.03.05, April 11, 2023-MRS Spring Meeting & Exhibit in San Francisco.

B. Rasulev, M. Zamani, S. Szwiec, G. Casanola-Martin, N. Fjodorova, M. Novič, K. Venko, M. Türker, G. Tugcu, S. Erdem, A. Toropova, A. Toropov.
Assessing Toxicity of Fullerene Nanostructures Using Human Proteins by Combined Computational Chemistry and Cheminformatics Approach.
https://www.mrs.org/meetings-events/spring-meetings-exhibits/2023-mrs-spring-meeting/call-for-papers/presentations/detail/2023_mrs_spring_meeting/3838685-202304110845

CORAL Freeware

A.A. Toropov, A.P. Toropova, E. Benfenati CORAL freeware (CORrelations And Logic) is available at http://www.insilico.eu/coral